UNIFORM ACCURACY OF EIGENPAIRS FROM A SHIFT-INVERT LANCZOS METHOD

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Abstract. This paper analyzes the accuracy of the shift-invert Lanczos iteration for computing the eigenpairs of the symmetric positive definite generalized eigenvalue problem that arises from a conforming finite element method. We provide bounds for the uniform (independent of the mesh size h) accuracy of the eigenpairs produced by shift-invert Lanczos given a residual reduction by exploiting the connection with the finite element method. We also discuss the implications of our analysis for practical shift-invert Lanczos iterations.

Key words. Shift-invert Lanczos decomposition, symmetric generalized eigenvalue problem, inner product

AMS subject classifications. 65F15, 65N25

1. Introduction. A popular approach for the solution of the generalized symmetric positive definite eigenvalue problem

$$\mathbf{Au} = \mathbf{Mu}\lambda, \quad \left(\mathbf{A}, \mathbf{M} \in \mathbb{R}^{n\times n}\right), \tag{1.1}$$

is the shift-invert Lanczos method [3, 4, 5]. The matrices $\mathbf{A}$ and $\mathbf{M}$ are symmetric and symmetric positive definite, respectively. This technique is used to approximate the eigenvalues in a given interval, for instance, the smallest eigenvalues.

Once approximations to the eigenvalues (and eigenvectors) are computed, a posteriori error bounds can assess the accuracy of the results. Ericsson and Ruhe [3] presented the first bounds for (1.1) when computing an $\mathbf{M}$-orthonormal Lanczos basis. In this paper, we review their results and extend them to an $(\mathbf{A} - \sigma\mathbf{M})$-orthonormal Lanczos basis (where σ is no larger than the smallest eigenvalue of $(\mathbf{A}, \mathbf{M})$).

The motivation for using the $(\mathbf{A} - \sigma\mathbf{M})$-inner product comes from the work of structural analysts who compute a large set of the smallest eigenpairs with one shift σ below the spectrum of $(\mathbf{A}, \mathbf{M})$. Indeed, when performing a series of factorizations becomes prohibitively expensive, preconditioned iterative methods replace the direct linear solves. These iterative methods perform at their best when $\mathbf{A} - \sigma\mathbf{M}$ is positive definite. Furthermore, when $\mathbf{A}$ is ill-conditioned or singular and $\mathbf{M}$ is ill-conditioned, there exists, in most cases, a shift σ so that $\mathbf{A} - \sigma\mathbf{M}$ is positive definite and better conditioned. This choice of σ helps not only the preconditioned iterative method but also in maintaining the orthonormality of Lanczos vectors. Our bounds indicate as well the attainable accuracy to eigenpairs of (1.1), when using a single shift.

Finally, when the eigenvalue problem (1.1) arises from the finite element discretization of elliptic self-adjoint differential eigenvalue problem, invariance of the bounds with respect to the mesh size is an important property. Our analysis studies the bounds with respect to the mesh size and also has implications on practical shift-invert Lanczos iterations.

Our paper is organized as follows. Section 2 reviews the shift-invert Lanczos decomposition and introduces our notation. Section 3 reviews useful accuracy results.

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Sections 4 and 5 provide accuracy results given a residual reduction achieved by the shift-invert Lanczos iteration. Finally, section 6 comments on the results of our analysis for practical Lanczos iterations.

2. Shift-invert Lanczos decomposition. The eigenvalue problem (1.1) has a set of $\mathbf{M}$-orthonormal eigenvectors $\mathbf{u}_j$ and corresponding eigenvalues λ_j. We assume that the eigenvalues (and eigenvectors) are ordered in ascending order.

In order to use the Lanczos iteration to compute eigenpairs of (1.1), a spectral transformation is employed. If $\sigma \in \mathbb{R}$, then the standard eigenvalue problem

$$(\mathbf{A} - \sigma\mathbf{M})^{-1}\mathbf{M}\mathbf{u} = \mathbf{u}\nu, \quad \left(\nu = \frac{1}{\lambda - \sigma}\right), \tag{2.1}$$

results by subtracting $\sigma\mathbf{M}$ from both sides of (1.1) followed by "cross-multiplication". This standard eigenvalue problem is no longer symmetric. However, a careful choice of inner product renders the operator $(\mathbf{A} - \sigma\mathbf{M})^{-1}\mathbf{M}$ symmetric. For instance, when the inner product is induced by the matrix $\mathbf{H}$, selecting $\mathbf{H}$ equal to $\mathbf{M}$ or $\mathbf{A} - \sigma\mathbf{M}$ ($\sigma < \lambda_1$) results in a $\mathbf{H}$-symmetric matrix $(\mathbf{A} - \sigma\mathbf{M})^{-1}\mathbf{M}$.

Suppose that

$$\mathbf{A}_\sigma^{-1}\mathbf{M}\mathbf{V}_j = \mathbf{V}_j\mathbf{T}_j + \mathbf{f}_j\mathbf{e}_j^T, \quad (\mathbf{A}_\sigma = \mathbf{A} - \sigma\mathbf{M}), \tag{2.2}$$

is a Lanczos reduction of length j where $\mathbf{e}_j$ is the jth canonical basis vector, we have

$$\mathbf{V}_j^T\mathbf{H}\mathbf{A}_\sigma^{-1}\mathbf{M}\mathbf{V}_j = \mathbf{T}_j \tag{2.3a}$$

$$\mathbf{V}_j^T\mathbf{H}\mathbf{V}_j = \mathbf{I}_j \tag{2.3b}$$

$$\mathbf{V}_j^T\mathbf{H}\mathbf{f}_j = \mathbf{0} \tag{2.3c}$$

where $\mathbf{T}_j$ is a symmetric tridiagonal matrix. The j columns of $\mathbf{V}_j$ form a basis $\mathbf{H}$-orthonormal for the Krylov subspace

$$\mathcal{K}_j(\mathbf{A}_\sigma^{-1}\mathbf{M}, \mathbf{v}_1) = \mathrm{Span}\{\mathbf{v}_1, \mathbf{A}_\sigma^{-1}\mathbf{M}\mathbf{v}_1, \cdots, (\mathbf{A}_\sigma^{-1}\mathbf{M})^{j-1}\mathbf{v}_1\}. \tag{2.4}$$

If we denote

$$\mathbf{T}_j = \begin{pmatrix} \alpha_1 & \beta_2 & \cdots & 0 \\ \beta_2 & \alpha_2 & \cdots & 0 \\ \vdots & & \ddots & \beta_j \\ 0 & \cdots & \beta_j & \alpha_j \end{pmatrix},$$

then the familiar Lanczos three-term recurrence is recovered by equating the jth column of (2.2) to obtain

$$\mathbf{f}_j = \mathbf{A}_\sigma^{-1}\mathbf{M}\mathbf{v}_j - \mathbf{v}_j\alpha_j - \mathbf{v}_{j-1}\beta_{j-1}.$$

Using $\mathbf{H}$-orthonormality, we have

$$\alpha_j = \mathbf{v}_j^T\mathbf{H}\mathbf{A}_\sigma^{-1}\mathbf{M}\mathbf{v}_j, \tag{2.5a}$$

$$\beta_{j+1} = \|\mathbf{f}_j\|_{\mathbf{H}}, \tag{2.5b}$$

and the new direction $\mathbf{v}_{j+1}$ is equal to $\mathbf{f}_j/\beta_{j+1}$.

The Lanczos reduction (2.2) provides two choices of approximating eigenvectors. If $\mathbf{T}_j\mathbf{s} = \mathbf{s}\theta$ where $\mathbf{s} \in \mathbb{R}^j, \theta \in \mathbb{R}$, and $\|\mathbf{s}\| = 1$, then we can postmultiply (2.2) by $\mathbf{s}$ to obtain

$$\mathbf{A}_\sigma^{-1}\mathbf{M}\mathbf{V}_j\mathbf{s} = \mathbf{V}_j\mathbf{s}\theta + \mathbf{f}_j\omega_j \tag{2.6a}$$

$$= (\mathbf{V}_j\mathbf{s} + \mathbf{f}_j\frac{\omega_j}{\theta})\theta, \tag{2.6b}$$

where $\omega_j = \mathbf{e}_j^T\mathbf{s}$. We define the Ritz vector as $\mathbf{x} = \mathbf{V}_j\mathbf{s}$ and the purified vector as $\mathbf{p} = \mathbf{x} + \mathbf{f}_j\omega_j/\theta$. The purified vector was introduced in [3, 6] as a simple postprocessing step to recover the vector that results from a step of inverse iteration on the Ritz vector.

For a desired tolerance ε, a convergence criterion often used in practice [3, 5] is

$$\|\mathbf{f}_j\|_\mathbf{H} |\omega_j| \le \varepsilon |\theta|. \tag{2.7}$$

Note that by (2.5b), the convergence criterion is available as a by-product of the Lanczos reduction.

In the remainder of this report, we omit the index j when the context is clear and we always assume that $\mathbf{A}_\sigma$ is invertible. We also emphasize that σ is smaller than λ_1 only when the inner product is induced by $\mathbf{H} = \mathbf{A}_\sigma$. Finally, we caution the reader that a distinction is drawn between the inner product used for orthogonality of the Lanczos vectors and the inner product used for the error bounds.

3. Useful general results. This section reviews a standard accuracy result that will prove useful for our analysis. We also introduce a useful lemma. This section concludes with some background information on the approximation of the finite element method to eigenvalues of the continuous problem that produced (1.1).

We recall the following result proved in Parlett [7, § 11.7]. The result provides bounds on the errors when approximating an eigenpair of (1.1) in terms of residuals.

THEOREM 3.1. *Let $\hat{\mathbf{A}} \in \mathbb{R}^{n\times n}$ be a symmetric matrix, $\hat{\mathbf{y}}(\neq \mathbf{0}) \in \mathbb{R}^n$ with Rayleigh quotient*

$$\hat{\theta} = \frac{\hat{\mathbf{y}}^T\hat{\mathbf{A}}\hat{\mathbf{y}}}{\hat{\mathbf{y}}^T\hat{\mathbf{y}}}$$

and residual $\hat{\mathbf{r}} = \hat{\mathbf{A}}\hat{\mathbf{y}} - \hat{\theta}\hat{\mathbf{y}}$. If $\hat{\alpha}$ is the eigenvalue of $\hat{\mathbf{A}}$ closest to $\hat{\theta}$ where $\hat{\mathbf{A}}\hat{\mathbf{z}} = \hat{\mathbf{z}}\hat{\alpha}$ and $\|\hat{\mathbf{z}}\| = 1$, then

$$0 \le \left|\hat{\theta} - \hat{\alpha}\right| \le \min\left(\frac{\|\hat{\mathbf{r}}\|}{\|\hat{\mathbf{y}}\|}, \frac{1}{\min\limits_{\hat{\lambda}_i\neq\hat{\alpha}}\left|\hat{\lambda}_i - \hat{\theta}\right|}\frac{\|\hat{\mathbf{r}}\|^2}{\|\hat{\mathbf{y}}\|^2}\right) \tag{3.1}$$

and

$$\frac{1}{\hat{\lambda}_n - \hat{\lambda}_1}\frac{\|\hat{\mathbf{r}}\|}{\|\hat{\mathbf{y}}\|} \le |\sin\angle(\hat{\mathbf{y}}, \hat{\mathbf{z}})| \le \frac{1}{\min\limits_{\hat{\lambda}_i\neq\hat{\alpha}}\left|\hat{\lambda}_i - \hat{\theta}\right|}\frac{\|\hat{\mathbf{r}}\|}{\|\hat{\mathbf{y}}\|}. \tag{3.2}$$

$\hat{\lambda}_n$ and $\hat{\lambda}_1$ are, respectively, the largest and smallest eigenvalue of $\hat{\mathbf{A}}$.

The following lemma relates the angle of a vector with an eigenvector using the $\mathbf{M}$- and $\mathbf{A}_\sigma$-inner products. We are not aware whether this result has appeared in the open literature.

LEMMA 3.2. *Let* $\sigma < \lambda_1$, $\mathbf{y}(\neq \mathbf{0}) \in \mathbb{R}^n$ *and*

$$\rho = \frac{\mathbf{y}^T\mathbf{A}\mathbf{y}}{\mathbf{y}^T\mathbf{M}\mathbf{y}}.$$

If $\mathbf{A}\mathbf{u} = \mathbf{M}\mathbf{u}\lambda$, *then*

$$\sin^2 \angle_{\mathbf{M}}(\mathbf{y}, \mathbf{u}) = \frac{\lambda - \rho}{\lambda - \sigma} + \frac{\rho - \sigma}{\lambda - \sigma} \sin^2 \angle_{\mathbf{A}_\sigma}(\mathbf{y}, \mathbf{u}). \tag{3.3}$$

Proof. The hypothesis implies $\mathbf{y}^T\mathbf{A}_\sigma\mathbf{u} = \mathbf{y}^T\mathbf{M}\mathbf{u}(\lambda - \sigma)$, $\mathbf{u}^T\mathbf{A}_\sigma\mathbf{u} = \mathbf{u}^T\mathbf{M}\mathbf{u}(\lambda - \sigma)$, and $\mathbf{y}^T\mathbf{A}_\sigma\mathbf{y} = \mathbf{y}^T\mathbf{M}\mathbf{y}(\rho - \sigma)$. Therefore we have

$$\frac{\mathbf{y}^T\mathbf{M}\mathbf{u}}{\|\mathbf{y}\|_{\mathbf{M}}\|\mathbf{u}\|_{\mathbf{M}}} = \sqrt{\frac{\rho - \sigma}{\lambda - \sigma}} \frac{\mathbf{y}^T\mathbf{A}_\sigma\mathbf{u}}{\|\mathbf{y}\|_{\mathbf{A}_\sigma}\|\mathbf{u}\|_{\mathbf{A}_\sigma}}.$$

The result follows from the identity $\cos^2 \phi + \sin^2 \phi = 1$. ☐

As we assume that the problem (1.1) arises from the discretization of a partial differential equation with a conforming finite element method, we could write (1.1) as

$$\mathbf{A}^h\mathbf{u}^h = \mathbf{M}^h\mathbf{u}^h\lambda^h, \tag{3.4}$$

where h is the characteristic mesh size. Our error bounds need to be uniform with respect to this mesh size. Theorem 3.1 uses the largest and smallest eigenvalues of $\hat{\mathbf{A}}$. So, for the sake of completeness, we recall a standard result from finite element theory [2]:

$$\lim_{h \to 0} \lambda_1^h = \lambda_1^\star, \quad \lim_{h \to 0} \lambda_n^h = +\infty, \tag{3.5}$$

where $\lambda_1^\star$ is the smallest eigenvalue of the differential eigenvalue problem. Note that $n \to +\infty$ as $h \to 0$. In the remainder of this report, we omit the subscript h.

4. Study of the Ritz vector. Using (2.6a), we approximate an eigenvector and corresponding eigenvalue by

$$\sigma + \frac{1}{\theta} = \sigma + \frac{\mathbf{x}^T\mathbf{H}\mathbf{x}}{\mathbf{x}^T\mathbf{H}\mathbf{A}_\sigma^{-1}\mathbf{M}\mathbf{x}}. \tag{4.1}$$

We remark that when $\mathbf{H}$ is equal to $\mathbf{A}_\sigma(\sigma < \lambda_1)$, the Rayleigh quotient of $\mathbf{x}$ for the pencil $(\mathbf{A}, \mathbf{M})$ is $\sigma + \theta^{-1}$. On the other hand, when the Lanczos vectors are $\mathbf{M}$-orthonormal, $\sigma + \theta^{-1}$ is not the Rayleigh quotient of $\mathbf{x}$ for the pencil $(\mathbf{A}, \mathbf{M})$. The next result relates the Lanczos vector $\mathbf{f}$ with the residual.

LEMMA 4.1. *If* $\mathbf{x}$ *is the Ritz vector (2.6a) produced by the Lanczos reduction, then*

$$\frac{\|\mathbf{A}\mathbf{x} - \mathbf{M}\mathbf{x}(\theta^{-1} + \sigma)\|_{\mathbf{A}_\sigma^{-1}\mathbf{H}\mathbf{A}_\sigma^{-1}}}{\|\mathbf{x}\|_{\mathbf{H}}} = \left|\frac{\omega}{\theta}\right| \|\mathbf{f}\|_{\mathbf{H}}. \tag{4.2}$$

Proof. The Ritz vector $\mathbf{x}$ is $\mathbf{H}$-normalized. Equation (2.6a) implies $\mathbf{A}_\sigma^{-1}(\mathbf{Mx} - \mathbf{A}_\sigma \mathbf{x}\theta) = \mathbf{f}\omega$ so that

$$\mathbf{A}_\sigma^{-1}(\mathbf{Ax} - \mathbf{Mx}(\theta^{-1} + \sigma)) = -\mathbf{f}\frac{\omega}{\theta},$$

which proves the relation (4.2). □

The following result combines (4.2) and Theorem 3.1 to provide bounds on the accuracy of the Ritz value and vector given by the shift-invert Lanczos reduction (2.2).

PROPOSITION 4.2. *Let $\mathbf{x}$ be a Ritz vector (2.6a) produced by a shift-invert Lanczos reduction and*

$$\theta = \frac{\mathbf{x}^T \mathbf{H} \mathbf{A}_\sigma^{-1} \mathbf{Mx}}{\mathbf{x}^T \mathbf{Hx}}.$$

If λ satisfies

$$\left| \frac{1}{\lambda - \sigma} - \theta \right| = \min_{\lambda_i} \left| \frac{1}{\lambda_i - \sigma} - \theta \right|$$

and $\mathbf{Au} = \mathbf{Mu}\lambda$ where $\|\mathbf{u}\|_{\mathbf{H}} = 1$ ($\sigma < \lambda_1$ when $\mathbf{H} = \mathbf{A}_\sigma$), then

$$\left| \frac{\lambda - \sigma - \theta^{-1}}{\lambda - \sigma} \right| \le \|\mathbf{f}\|_{\mathbf{H}} \left| \frac{\omega}{\theta} \right| \min\left(1, \left| \frac{\lambda_{gap} - \sigma}{\lambda_{gap} - \sigma - \theta^{-1}} \right| \|\mathbf{f}\|_{\mathbf{H}} \left| \frac{\omega}{\theta} \right| \right) \tag{4.3}$$

and

$$\left| \frac{(\lambda_\sigma^+ - \sigma)(\lambda_\sigma^- - \sigma)}{\lambda_\sigma^+ - \lambda_\sigma^-} \right| \|\mathbf{f}\|_{\mathbf{H}} |\omega| \le |\sin \angle_{\mathbf{H}}(\mathbf{x}, \mathbf{u})| \le \left| \frac{\lambda_{gap} - \sigma}{\lambda_{gap} - \sigma - \theta^{-1}} \right| \|\mathbf{f}\|_{\mathbf{H}} \left| \frac{\omega}{\theta} \right| \tag{4.4}$$

where

$$\left| \frac{1}{\lambda_{gap} - \sigma} - \theta \right| = \min_{\lambda_i \neq \lambda} \left| \frac{1}{\lambda_i - \sigma} - \theta \right|$$

and

$$(\lambda_\sigma^-, \lambda_\sigma^+) = \begin{cases} (\min_{\lambda_i < \sigma} |\lambda_i - \sigma|, \min_{\sigma < \lambda_i} |\lambda_i - \sigma|) & \text{when } \lambda_1 < \sigma < \lambda_n, \\ (\lambda_1, \lambda_n) & \text{otherwise.} \end{cases}$$

Proof. This result is a reformulation of Theorem 3.1 when $\hat{\mathbf{A}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{r}}$ are respectively equal to $\mathbf{H}^{1/2}\mathbf{A}_\sigma^{-1}\mathbf{M}\mathbf{H}^{-1/2}$, $\mathbf{H}^{1/2}\mathbf{x}$, and $\theta\mathbf{H}^{1/2}\mathbf{A}_\sigma^{-1}(\mathbf{Mx}(\theta^{-1} + \sigma) - \mathbf{Ax})$. $\hat{\alpha}$ and $\hat{\lambda}_i$ are equal to $1/(\lambda - \sigma)$ and $1/(\lambda_i - \sigma)$. The Rayleigh quotient of $\hat{\mathbf{y}}$ coincides with θ. The bounds (4.3) and (4.4) then follow by using (4.2). □

We remark that Proposition 4.2 is only related to the shift-invert Lanczos method via the relation (4.2) and as soon as the convergence criterion (2.7) is satisfied, we can introduce the tolerance ε in the upper bounds.

The eigenvalue bound (4.3) shows that when σ is close to λ, a large tolerance ε can still result in an accurate approximation of the eigenvalue. The bound also guarantees a relative error on the eigenvalue of the same level as the residual norm (4.2). Finally, a quadratic convergence is triggered as soon as

$$\left| \frac{\lambda_{gap} - \sigma}{\lambda_{gap} - \sigma - \theta^{-1}} \right| \|\mathbf{f}\|_{\mathbf{H}} \left| \frac{\omega}{\theta} \right| < 1.$$

When approximating many eigenpairs with one shift σ, $|\theta|$ becomes smaller and $|\lambda_{gap} - \sigma|$ larger. Therefore, the ratio between the sine of the angle and the residual norm (4.2)

$$\left| \frac{(\lambda_\sigma^+ - \sigma)(\lambda_\sigma^- - \sigma)}{\lambda_\sigma^+ - \lambda_\sigma^-} \right| |\theta| \leq \frac{|\sin \angle_{\mathbf{H}}(\mathbf{x}, \mathbf{u})|}{\|\mathbf{A}\mathbf{x} - \mathbf{M}\mathbf{x}(\theta^{-1} + \sigma)\|_{\mathbf{A}_\sigma^{-1}\mathbf{H}\mathbf{A}_\sigma^{-1}}} \leq \left| \frac{\lambda_{gap} - \sigma}{\lambda_{gap} - \sigma - \theta^{-1}} \right|$$

belongs to a wider interval.

The discussion at the end of section 3 implies that the sharpness of bounds (4.3) and (4.4) are invariant with respect to the mesh size. However, when using the **M**-inner product, the Rayleigh quotient of the Ritz vector $\mathbf{x}$ does not remain bounded with the mesh size. Indeed, the Lanczos reduction (2.2) implies

$$\mathbf{M}\mathbf{x} = \mathbf{A}_\sigma \mathbf{x}\theta + \mathbf{A}_\sigma \mathbf{f}\omega,$$

which gives

$$\begin{aligned} \mathbf{x}^T\mathbf{M}\mathbf{x} &= (\mathbf{x}^T\mathbf{A}\mathbf{x} - \sigma\mathbf{x}^T\mathbf{M}\mathbf{x})\theta + (\mathbf{x}^T\mathbf{A}\mathbf{f} - \sigma\mathbf{x}^T\mathbf{M}\mathbf{f})\omega, \\ \mathbf{f}^T\mathbf{M}\mathbf{x} &= (\mathbf{f}^T\mathbf{A}\mathbf{x} - \sigma\mathbf{f}^T\mathbf{M}\mathbf{x})\theta + (\mathbf{f}^T\mathbf{A}\mathbf{f} - \sigma\mathbf{f}^T\mathbf{M}\mathbf{f})\omega. \end{aligned} \tag{4.5}$$

Because $\mathbf{f}$ is **M**-orthogonal to the Ritz vector $\mathbf{x}$, we obtain

$$\frac{\mathbf{x}^T\mathbf{A}\mathbf{x}}{\mathbf{x}^T\mathbf{M}\mathbf{x}} = \sigma + \frac{1}{\theta} + \left(\frac{\mathbf{f}^T\mathbf{A}\mathbf{f}}{\mathbf{f}^T\mathbf{M}\mathbf{f}} - \sigma \right) \left(\|\mathbf{f}\|_{\mathbf{M}} \frac{\omega}{\theta} \right)^2 .$$

This equality implies that the Rayleigh quotient of $\mathbf{x}$ for the pencil $(\mathbf{A}, \mathbf{M})$ is bounded with the mesh size only when the Rayleigh quotient of $\mathbf{f}$ for the pencil $(\mathbf{A}, \mathbf{M})$ remains bounded. The following example demonstrates that these Rayleigh quotients can grow when the mesh is refined.

Consider the $(2n-1) \times (2n-1)$ tridiagonal matrices

$$\mathbf{A} = 2n \begin{pmatrix} 2 & -1 & \cdots & 0 \\ -1 & 2 & \cdots & 0 \\ \vdots & & \ddots & -1 \\ 0 & \cdots & -1 & 2 \end{pmatrix}, \quad \mathbf{M} = \frac{1}{12n} \begin{pmatrix} 4 & 1 & \cdots & 0 \\ 1 & 4 & \cdots & 0 \\ \vdots & & \ddots & 1 \\ 0 & \cdots & 1 & 4 \end{pmatrix},$$

that arise from a uniform finite element discretization of the Laplace equation with homogeneous Dirichlet boundary conditions on the unit interval. A shift-invert Lanczos iteration with an **M**-inner product is used to approximate the smallest eigenpair. The starting vector is **M**-normalized and proportional to $\mathbf{e}_n$. The Ritz vector $\mathbf{x}$ is obtained as soon as the stopping criterion (2.7) is satisfied with $\varepsilon = 10^{-2}$. Figure 4.1 demonstrates that the Rayleigh quotient of $\mathbf{x}$ for the pencil ($\mathbf{A}$, $\mathbf{M}$) grows as we refine the mesh. Consequently, the accuracy of the Ritz vector, defined by the Lanczos reduction with **M**-inner product, decreases with the mesh size. On the other hand, using the $\mathbf{A}_\sigma$-inner product results in a bounded Rayleigh quotient for $\mathbf{x}$, equal to $\sigma + \theta^{-1}$.

5. Study of the purified vector. This section studies the case when the eigenpair is approximated by the purified vector (2.6b) and the corresponding Rayleigh quotient. We consider the two cases that arise when the Lanczos vectors are orthonormal with respect to the **M**- and $\mathbf{A}_\sigma$-inner products.

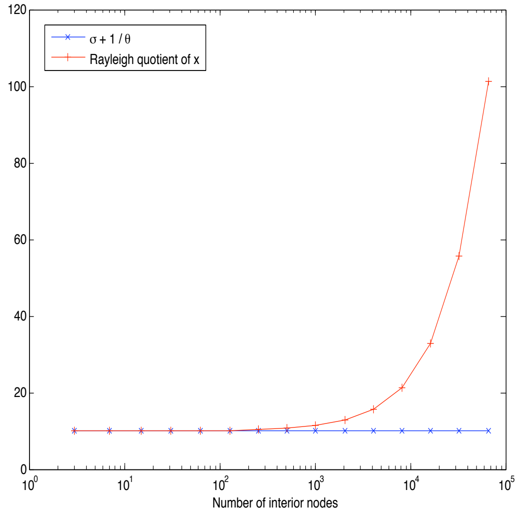

FIG. 4.1. *Size of the Rayleigh quotient with mesh refinement* ($\varepsilon = 10^{-2}$) *using an* $\mathbf{M}$-*orthonormal shift-invert Lanczos method.*

5.1. Lanczos reduction with M-inner product. The following result is a counterpart of Lemma 4.1.

LEMMA 5.1. *If* $\mathbf{p}$ *is the purified vector (2.6b) given by the shift-invert Lanczos reduction (2.2) where the Lanczos vectors are* $\mathbf{M}$-*orthonormal, then*

$$\rho = \frac{\mathbf{p}^T\mathbf{A}\mathbf{p}}{\mathbf{p}^T\mathbf{M}\mathbf{p}} = \sigma + \frac{1}{\theta(1+\|\mathbf{f}\|_{\mathbf{M}}^2(\omega/\theta)^2)}, \tag{5.1}$$

$$\frac{\|\mathbf{r}\|_{\mathbf{M}^{-1}}}{\|\mathbf{p}\|_{\mathbf{M}}} = |\rho-\sigma|\,\|\mathbf{f}\|_{\mathbf{M}}\left|\frac{\omega}{\theta}\right| = \|\mathbf{f}\|_{\mathbf{M}}\frac{|\omega|}{\theta^2}\times\frac{1}{1+\|\mathbf{f}\|_{\mathbf{M}}^2(\omega/\theta)^2}, \tag{5.2}$$

$$\frac{\|\mathbf{r}\|_{\mathbf{A}_\mu^{-1}}}{\|\mathbf{p}\|_{\mathbf{A}_\mu}} = \frac{1}{\sqrt{\rho-\mu}}\|\mathbf{f}\|_{\mathbf{M}\mathbf{A}_\mu^{-1}\mathbf{M}}\frac{|\omega|}{\theta^2} + \mathcal{O}\left(\|\mathbf{f}\|_{\mathbf{M}}^2\left(\frac{\omega}{\theta}\right)^2\right), \tag{5.3}$$

where $\mathbf{r} = \mathbf{A}\mathbf{p} - \mathbf{M}\mathbf{p}\rho$ *denotes the residual,* $\|\mathbf{f}\|_{\mathbf{M}}\,|\omega/\theta| < 1$, *and* μ *is smaller than* λ_1 *such that* $\mathbf{A}_\mu$ *is positive definite.*

Proof. The two results (5.1) and (5.2) are due to Ericsson and Ruhe [3]. The Lanczos reduction (2.2) implies

$$\mathbf{r} = \mathbf{A}\mathbf{p} - (\sigma+\frac{1}{\theta})\mathbf{M}\mathbf{p} + (\sigma+\frac{1}{\theta}-\rho)\mathbf{M}\mathbf{p} = -\mathbf{M}\mathbf{f}\frac{\omega}{\theta^2} + (\sigma+\frac{1}{\theta}-\rho)\mathbf{M}\mathbf{p}.$$

so that

$$\mathbf{r}^T\mathbf{A}_\mu^{-1}\mathbf{r} = \mathbf{f}^T\mathbf{M}\mathbf{A}_\mu^{-1}\mathbf{M}\mathbf{f}\left(\frac{\omega}{\theta^2}\right)^2 - \mathbf{f}^T\mathbf{M}\mathbf{A}_\mu^{-1}\mathbf{M}\mathbf{p}\frac{2\gamma\omega}{\theta^2} + \mathbf{p}^T\mathbf{M}\mathbf{A}_\mu^{-1}\mathbf{M}\mathbf{p}\gamma^2,$$

where $\gamma = \sigma - \rho + \theta^{-1}$. The following relations

$$\begin{cases} \mathbf{p}^T\mathbf{M}\mathbf{A}_\mu^{-1}\mathbf{M}\mathbf{p} \le \dfrac{1}{\lambda_1-\mu}\mathbf{p}^T\mathbf{M}\mathbf{p} = \dfrac{1+\|\mathbf{f}\|_\mathbf{M}^2(\omega/\theta)^2}{\lambda_1-\mu}, \\ \sigma + \dfrac{1}{\theta} - \rho = \dfrac{\|\mathbf{f}\|_\mathbf{M}^2(\omega/\theta)^2}{\theta(1+\|\mathbf{f}\|_\mathbf{M}^2(\omega/\theta)^2)}, \\ \mathbf{f}^T\mathbf{M}\mathbf{A}_\mu^{-1}\mathbf{M}\mathbf{p} = \mathbf{f}^T\mathbf{M}\mathbf{A}_\mu^{-1}\mathbf{M}\mathbf{x} + \mathbf{f}^T\mathbf{M}\mathbf{A}_\mu^{-1}\mathbf{M}\mathbf{f}\dfrac{\omega}{\theta}, \\ \mathbf{M}\mathbf{A}_\mu^{-1}\mathbf{M}\mathbf{x} = \mathbf{M}\mathbf{x}\theta + \mathbf{M}\mathbf{A}_\mu^{-1}\mathbf{M}\mathbf{x}\theta(\mu-\sigma) + \mathbf{M}\mathbf{f}\omega + \mathbf{M}\mathbf{A}_\mu^{-1}\mathbf{M}\mathbf{f}\omega(\mu-\sigma), \end{cases}$$

show that

$$\|\mathbf{r}\|_{\mathbf{A}_\mu^{-1}} = \|\mathbf{f}\|_{\mathbf{M}\mathbf{A}_\mu^{-1}\mathbf{M}}\frac{|\omega|}{\theta^2} + \mathcal{O}\left(\|\mathbf{f}\|_\mathbf{M}^2\left(\frac{\omega}{\theta}\right)^2\right).$$

The result (5.3) now follows because

$$\mathbf{p}^T\mathbf{A}_\mu\mathbf{p} = (\rho-\mu)\left(1+\|\mathbf{f}\|_\mathbf{M}^2\left(\frac{\omega}{\theta}\right)^2\right).$$

□

We remark that $\rho < \sigma + 1/\theta$. In general, σ is arbitrary. However, when σ is smaller than λ_1, we can set μ to σ and we have $\|\mathbf{f}_j\|_{\mathbf{M}\mathbf{A}_\sigma^{-1}\mathbf{M}} = \beta_{j+1}\sqrt{\alpha_{j+1}}$ by (2.5). The following result combines Lemma 5.1 and Theorem 3.1 to provide accuracy bounds.

PROPOSITION 5.2. *Let* $\mathbf{p}$ *be the purified vector (2.6b) given by the shift-invert Lanczos reduction (2.2) with the* $\mathbf{M}$*-inner product,* ρ *its Rayleigh quotient, and* $\mathbf{r} = \mathbf{A}\mathbf{p} - \mathbf{M}\mathbf{p}\rho$*. If* $\mu < \lambda_1$ *and* $\mathbf{A}\mathbf{u} = \mathbf{M}\mathbf{u}\lambda$ *where* λ *is the closest eigenvalue to* ρ*, then*

$$\left|\frac{\lambda-\rho}{\rho}\right| \le \frac{1}{\rho}\frac{\|\mathbf{r}\|_{\mathbf{M}^{-1}}}{\|\mathbf{p}\|_\mathbf{M}}\min\left(1, \frac{1}{\min\limits_{\lambda_i\neq\lambda}|\lambda_i-\rho|}\frac{\|\mathbf{r}\|_{\mathbf{M}^{-1}}}{\|\mathbf{p}\|_\mathbf{M}}\right) \tag{5.4a}$$

$$\left|\frac{\lambda-\rho}{\lambda-\mu}\right| \le \frac{\|\mathbf{r}\|_{\mathbf{A}_\mu^{-1}}}{\|\mathbf{p}\|_{\mathbf{A}_\mu}}\min\left(1, \left|\frac{\lambda_{gap}-\mu}{\lambda_{gap}-\rho}\right|\frac{\|\mathbf{r}\|_{\mathbf{A}_\mu^{-1}}}{\|\mathbf{p}\|_{\mathbf{A}_\mu}}\right) \tag{5.4b}$$

and

$$\frac{1}{\lambda_n-\lambda_1}\frac{\|\mathbf{r}\|_{\mathbf{M}^{-1}}}{\|\mathbf{p}\|_\mathbf{M}} \le |\sin\angle_\mathbf{M}(\mathbf{p},\mathbf{u})| \le \frac{1}{\min\limits_{\lambda_i\neq\lambda}|\lambda_i-\lambda|}\frac{\|\mathbf{r}\|_{\mathbf{M}^{-1}}}{\|\mathbf{p}\|_\mathbf{M}} \tag{5.5a}$$

$$\frac{(\lambda_1-\mu)(\lambda_n-\mu)}{(\lambda_n-\lambda_1)(\rho-\mu)}\frac{\|\mathbf{r}\|_{\mathbf{A}_\mu^{-1}}}{\|\mathbf{p}\|_{\mathbf{A}_\mu}} \le \left|\sin\angle_{\mathbf{A}_\mu}(\mathbf{p},\mathbf{u})\right| \le \left|\frac{\lambda_{gap}-\mu}{\lambda_{gap}-\rho}\right|\frac{\|\mathbf{r}\|_{\mathbf{A}_\mu^{-1}}}{\|\mathbf{p}\|_{\mathbf{A}_\mu}} \tag{5.5b}$$

where λ_{gap} *satisfies*

$$\left|\frac{1}{\lambda_{gap}-\mu} - \frac{1}{\rho-\mu}\right| = \min_{\lambda_i\neq\lambda}\left|\frac{1}{\lambda_i-\mu} - \frac{1}{\rho-\mu}\right|.$$

Proof. This result is a reformulation of Theorem 3.1. For relations (5.4a) and (5.5a), $\hat{\mathbf{A}}$, $\hat{\mathbf{y}}$, and $\hat{\theta}$ are equal, respectively, to $\mathbf{M}^{-1/2}\mathbf{A}\mathbf{M}^{-1/2}$, $\mathbf{M}^{1/2}\mathbf{p}$, and ρ. To prove (5.4b) and (5.5b), they are equal, respectively, to $\mathbf{A}_\mu^{-1/2}\mathbf{M}\mathbf{A}_\mu^{-1/2}$, $\mathbf{A}_\mu^{1/2}\mathbf{p}$, and $1/(\rho-\mu)$. ◻

When the problem (1.1) arises from a finite element method, the bounds (5.4) and (5.5b) are uniform with the mesh size. However, the discussion at the end of section 3 implies that the lower bound of (5.5a) is not uniform with the mesh size.

As soon as the convergence criterion (2.7) is satisfied, we can introduce the tolerance ε in the bounds of Proposition 5.2. In particular, we can assume

$$\frac{\|\mathbf{r}\|_{\mathbf{M}^{-1}}}{\|\mathbf{p}\|_{\mathbf{M}}} \approx \frac{\varepsilon}{|\theta|}.$$

So when σ is close to λ, $|\theta|$ is large and a large tolerance ε can still result in an accurate approximation of λ and a small angle $\angle_{\mathbf{M}}(\mathbf{p},\mathbf{u})$. On the other hand, when $|\theta|$ is small, the bound (5.4a) guarantees at least a relative error close to ε but the upper bound of (5.5a) grows.

5.2. Lanczos reduction with $\mathbf{A}_\sigma$-inner product. The following result is a counterpart of Lemmas 4.1 and 5.1.

LEMMA 5.3. *If $\mathbf{p}$ is the purified vector (2.6b) given by the Lanczos reduction (2.2) where the Lanczos vectors are $\mathbf{A}_\sigma$-orthonormal ($\sigma < \lambda_1$), then*

$$\rho = \frac{\mathbf{p}^T\mathbf{A}\mathbf{p}}{\mathbf{p}^T\mathbf{M}\mathbf{p}} = \sigma + \frac{1}{\theta}\frac{1+\|\mathbf{f}\|^2_{\mathbf{A}_\sigma}(\omega/\theta)^2}{1+2\|\mathbf{f}\|^2_{\mathbf{A}_\sigma}(\omega/\theta)^2+\theta^{-1}\|\mathbf{f}\|^2_{\mathbf{M}}(\omega/\theta)^2}, \tag{5.6}$$

$$\frac{\|\mathbf{r}\|_{\mathbf{M}^{-1}}}{\|\mathbf{p}\|_{\mathbf{M}}} = \|\mathbf{f}\|_{\mathbf{M}}\frac{|\omega|}{\theta^{5/2}} + \mathcal{O}\left(\|\mathbf{f}\|^2_{\mathbf{A}_\sigma}\left(\frac{\omega}{\theta}\right)^2\right), \tag{5.7}$$

$$\frac{\|\mathbf{r}\|_{\mathbf{A}_\sigma^{-1}}}{\|\mathbf{p}\|_{\mathbf{A}_\sigma}} = \|\mathbf{f}\|_{\mathbf{M}\mathbf{A}_\sigma^{-1}\mathbf{M}}\frac{|\omega|}{\theta^2} + \mathcal{O}\left(\|\mathbf{f}\|^2_{\mathbf{A}_\sigma}\left(\frac{\omega}{\theta}\right)^2\right), \tag{5.8}$$

where $\mathbf{r} = \mathbf{A}\mathbf{p} - \mathbf{M}\mathbf{p}\rho$ *denotes the residual and* $\|\mathbf{f}\|_{\mathbf{A}_\sigma}|\omega/\theta| < 1$.

Proof. The definition of $\mathbf{A}_\sigma$ implies that

$$\mathbf{p}^T\mathbf{A}\mathbf{p} = \mathbf{p}^T\mathbf{A}_\sigma\mathbf{p} + \sigma\mathbf{p}^T\mathbf{M}\mathbf{p},$$
$$\mathbf{p}^T\mathbf{A}\mathbf{p} = 1 + \|\mathbf{f}\|^2_{\mathbf{A}_\sigma}\left(\frac{\omega}{\theta}\right)^2 + \sigma\mathbf{p}^T\mathbf{M}\mathbf{p},$$

where we have used (2.6b) and the $\mathbf{A}_\sigma$-orthogonality between $\mathbf{f}$ and the $\mathbf{A}_\sigma$-normalized vector $\mathbf{x}$.

The Lanczos reduction (2.2) implies $\mathbf{x}^T\mathbf{M}\mathbf{x} = \theta$ and $\mathbf{x}^T\mathbf{M}\mathbf{f} = \mathbf{f}^T\mathbf{A}_\sigma\mathbf{f}\omega$ so that

$$\mathbf{p}^T\mathbf{M}\mathbf{p} = \mathbf{x}^T\mathbf{M}\mathbf{x} + 2\mathbf{x}^T\mathbf{M}\mathbf{f}\frac{\omega}{\theta} + \mathbf{f}^T\mathbf{M}\mathbf{f}\left(\frac{\omega}{\theta}\right)^2,$$
$$\mathbf{p}^T\mathbf{M}\mathbf{p} = \theta\left[1 + 2\|\mathbf{f}\|^2_{\mathbf{A}_\sigma}\left(\frac{\omega}{\theta}\right)^2 + \frac{1}{\theta}\|\mathbf{f}\|^2_{\mathbf{M}}\left(\frac{\omega}{\theta}\right)^2\right],$$

and (5.6) is established.

The proofs of (5.7) and (5.8) are similar to that used to establish (5.3). Again, the Lanczos reduction (2.2) implies

$$\mathbf{r} = -\mathbf{M}\mathbf{f}\frac{\omega}{\theta^2} + (\sigma + \frac{1}{\theta} - \rho)\mathbf{M}\mathbf{p},$$

so that

$$\mathbf{r}^T\mathbf{M}^{-1}\mathbf{r} = \mathbf{f}^T\mathbf{M}\mathbf{f}\left(\frac{\omega}{\theta^2}\right)^2 - \mathbf{f}^T\mathbf{M}\mathbf{p}\frac{2\gamma\omega}{\theta^2} + \mathbf{p}^T\mathbf{M}\mathbf{p}\gamma^2,$$

where $\gamma = \sigma - \rho + \theta^{-1}$. The following relations,

$$\begin{cases} \mathbf{p}^T\mathbf{M}\mathbf{p} = \theta\left[1 + 2\|\mathbf{f}\|^2_{\mathbf{A}_\sigma}\left(\frac{\omega}{\theta}\right)^2 + \frac{1}{\theta}\|\mathbf{f}\|^2_{\mathbf{M}}\left(\frac{\omega}{\theta}\right)^2\right], \\ \\ \|\mathbf{f}\|^2_{\mathbf{M}} \le \frac{1}{\lambda_1 - \sigma}\|\mathbf{f}\|^2_{\mathbf{A}_\sigma}, \\ \\ \sigma + \frac{1}{\theta} - \rho = \mathcal{O}\left(\|\mathbf{f}\|^2_{\mathbf{A}_\sigma}\left(\frac{\omega}{\theta}\right)^2\right), \\ \\ \mathbf{f}^T\mathbf{M}\mathbf{p} = \mathbf{f}^T\mathbf{M}\mathbf{x} + \mathbf{f}^T\mathbf{M}\mathbf{f}\frac{\omega}{\theta} = \mathbf{f}^T\mathbf{A}_\sigma\mathbf{f}\omega + \mathbf{f}^T\mathbf{M}\mathbf{f}\frac{\omega}{\theta}, \end{cases}$$

establish (5.7) and (5.8) follows in a similar fashion. ∎

We remark that $\|\mathbf{f}\|_{\mathbf{M}}$ is available as a by-product of the Lanczos reduction through the relation (2.5). In contrast, $\|\mathbf{f}\|_{\mathbf{M}\mathbf{A}_\sigma^{-1}\mathbf{M}}$ is not. The following result combines Lemma 5.3 and Theorem 3.1 to provide accuracy bounds.

PROPOSITION 5.4. *Let* $\mathbf{p}$ *be the purified vector (2.6b) given by the shift-invert Lanczos reduction (2.2) with the* $\mathbf{A}_\sigma$*-inner product,* ρ *its Rayleigh quotient, and* $\mathbf{r} = \mathbf{A}\mathbf{p} - \mathbf{M}\mathbf{p}\rho$*. If* $\mathbf{A}\mathbf{u} = \mathbf{M}\mathbf{u}\lambda$ *where* λ *is the closest eigenvalue to* ρ*, then*

$$\left|\frac{\lambda - \rho}{\rho}\right| \le \frac{1}{\rho}\frac{\|\mathbf{r}\|_{\mathbf{M}^{-1}}}{\|\mathbf{p}\|_{\mathbf{M}}}\min\left(1, \frac{1}{\min\limits_{\lambda_i \ne \lambda}|\lambda_i - \rho|}\frac{\|\mathbf{r}\|_{\mathbf{M}^{-1}}}{\|\mathbf{p}\|_{\mathbf{M}}}\right) \tag{5.9a}$$

$$\left|\frac{\lambda - \rho}{\lambda - \sigma}\right| \le \frac{\|\mathbf{r}\|_{\mathbf{A}_\sigma^{-1}}}{\|\mathbf{p}\|_{\mathbf{A}_\sigma}}\min\left(1, \left|\frac{\lambda_{gap} - \sigma}{\lambda_{gap} - \rho}\right|\frac{\|\mathbf{r}\|_{\mathbf{A}_\sigma^{-1}}}{\|\mathbf{p}\|_{\mathbf{A}_\sigma}}\right) \tag{5.9b}$$

and

$$\frac{1}{\lambda_n - \lambda_1}\frac{\|\mathbf{r}\|_{\mathbf{M}^{-1}}}{\|\mathbf{p}\|_{\mathbf{M}}} \le |\sin\angle_{\mathbf{M}}(\mathbf{p}, \mathbf{u})| \le \frac{1}{\min\limits_{\lambda_i \ne \lambda}|\lambda_i - \lambda|}\frac{\|\mathbf{r}\|_{\mathbf{M}^{-1}}}{\|\mathbf{p}\|_{\mathbf{M}}} \tag{5.10a}$$

$$\frac{(\lambda_1 - \sigma)(\lambda_n - \sigma)}{(\lambda_n - \lambda_1)(\rho - \sigma)}\frac{\|\mathbf{r}\|_{\mathbf{A}_\sigma^{-1}}}{\|\mathbf{p}\|_{\mathbf{A}_\sigma}} \le |\sin\angle_{\mathbf{A}_\sigma}(\mathbf{p}, \mathbf{u})| \le \left|\frac{\lambda_{gap} - \sigma}{\lambda_{gap} - \rho}\right|\frac{\|\mathbf{r}\|_{\mathbf{A}_\sigma^{-1}}}{\|\mathbf{p}\|_{\mathbf{A}_\sigma}} \tag{5.10b}$$

where λ_{gap} *satisfies*

$$\left|\frac{1}{\lambda_{gap} - \sigma} - \frac{1}{\rho - \sigma}\right| = \min_{\lambda_i \ne \lambda}\left|\frac{1}{\lambda_i - \sigma} - \frac{1}{\rho - \sigma}\right|.$$

Proof. The proof is similar to the one for Proposition 5.2. ∎

The remarks following Proposition 5.2 remain valid. As soon as the convergence criterion (2.7) is satisfied, we can introduce the tolerance ε in the bounds of Proposition 5.4, using the relations

$$\|\mathbf{f}\|_{\mathbf{M}\mathbf{A}_\sigma^{-1}\mathbf{M}} \le \frac{1}{\sqrt{\lambda_1 - \sigma}}\|\mathbf{f}\|_{\mathbf{M}} \le \frac{1}{\lambda_1 - \sigma}\|\mathbf{f}\|_{\mathbf{A}_\sigma}.$$

6. Practical shift-invert Lanczos iterations. Our analysis indicates that the purified vector and its associated Rayleigh quotient are to be preferred over the Ritz vector. Indeed, the purified vector $\mathbf{p} = \mathbf{V}\mathbf{s} + \mathbf{f}\omega/\theta$ is richer than the Ritz vector $\mathbf{x} = \mathbf{V}\mathbf{s}$. Moreover, regardless of whether we use the $\mathbf{M}$- or $\mathbf{A}_\sigma$-inner product to maintain orthogonality of the Lanczos vectors, the Rayleigh quotient of the purified vector is invariant as the mesh is refined.

The paper [1] shows that the tolerance for the eigensolver can be set at the level of discretization error. When using large values for ε, say 10^{-3}-10^{-5}, purified vectors may not be $\mathbf{H}$-orthogonal to working precision when the purified residuals are of comparable size because

$$\left|\mathbf{p}^T\mathbf{H}\mathbf{q}\right| = \|\mathbf{f}\|_{\mathbf{H}}^2 \left|\frac{\mathbf{e}^T\mathbf{s}_{\mathbf{p}}}{\theta_{\mathbf{p}}}\right| \left|\frac{\mathbf{e}^T\mathbf{s}_{\mathbf{q}}}{\theta_{\mathbf{q}}}\right| \leq \varepsilon^2.$$

One easy solution is to perform, as post-processing, a Rayleigh-Ritz analysis for the pencil $(\mathbf{A}, \mathbf{M})$ and the space spanned by $\mathbf{V}$ and $\mathbf{f}$. When $\mathbf{H}$ is equal to $\mathbf{M}$, the construction of projected matrices is described in [6]. When $\mathbf{H}$ is equal to $\mathbf{A}_\sigma$ ($\sigma < \lambda_1$), the projected matrices are available as by-products of the Lanczos reduction. This extra Rayleigh-Ritz step will restore the $\mathbf{M}$-orthonormality and improve the approximation of eigenpairs.

In this paper, we draw a distinction between the inner product used for orthogonality of the Lanczos vectors and the inner product used for the error bounds. When measuring the residual with the $\mathbf{M}^{-1}$-norm, the accuracy bounds are not uniform with respect to the mesh size. On the other hand, when μ is smaller than λ_1, using the $\mathbf{A}_\mu^{-1}$-norm for measuring residuals results in uniform bounds. To build a Lanczos basis, the $\mathbf{M}$-inner product is appropriate when $\mathbf{M}$ is well conditioned. Otherwise, the $\mathbf{A}_\sigma$-inner product is a viable alternative for maintaining the orthonormality of the Lanczos vectors and can help a preconditioned iterative method ($\sigma < \lambda_1$).

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